Sodalite Network: Height and Spherical Content (Coordination Sequence)

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Abstract

The *sodalite* network is the edge-skeleton of the uniform tiling in Euclidean 3-dimensional space by Archimedean tetrakaidecahedra (truncated octahedra). We develop explicit expressions for its *height* (minimum network path length from some fixed to given vertex) and *coordination* (content of network sphere of given height) functions. The final discussion should to some extent assist in motivating and signposting our proof strategy, in the course of ruminating on its potential generalisation.

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1 Geometry and Symmetry

The *sodalite* network is the edge-skeleton of the uniform tiling in Euclidean 3-dimensional space by Archimedean tetrakaidecahedra (truncated octahedra). It may be constructed by 'bitruncating' vertices of the standard cubical tiling, so that octahedra forming around cubical vertices collide and in turn become truncated.

After scaling up by a factor 4, the canonical cell centred (around a cubical vertex) at origin $(0, 0, 0)$ has 24 vertices

$$\begin{gathered}\{(0,1,2),\ (0,2,1),\ (2,0,1),\ (2,1,0),\ (1,2,0),\ (1,0,2),\\ (0,-1,2),\ (0,2,-1),\ (2,0,-1),\ (2,-1,0),\ (-1,2,0),\ (-1,0,2),\\ (0,-1,-2),\ (0,-2,-1),\ (-2,0,-1),\ (-2,-1,0),\ (-1,-2,0),\ (-1,0,-2),\\ (0,1,-2),\ (0,-2,1),\ (-2,0,1),\ (-2,1,0),\ (1,-2,0),\ (1,0,-2)\},\end{gathered} \tag{1}$$

generated by the octahedral group $\mathcal{O}_3$ acting on the canonical vertex $O = (0, 1, 2)$. A useful rule of thumb is that $P = (x, y, z)$ represents a network vertex just when none of the 6 sums or differences of pairs of integer components vanishes:

$$x \pm y,\ y \pm z,\ z \pm x \neq 0 \pmod 4. \tag{2}$$

Each vertex P has four network neighbours, at Euclidean separation $\sqrt{2}$; the neighbours of $O = (0,1,2)$ comprise

$$\{(0,2,1), (0,2,3), (1,0,2), (-1,0,2)\}. \tag{3}$$

A *sector* denotes any of 48 isomorphs of the canonical fundamental region

$$\mathcal{U} \equiv \{(x,y,z) \mid x \geq y \geq z \geq 0\} \tag{4}$$

under the action of $\mathcal{O}_3$. To any vertex $P = (x,y,z)$ corresponds an isomorph $P' = (x',y',z') \in \mathcal{U}$, where x',y',z' denotes the same bag of integers as x,y,z, apart from dropping signs and sorting. Remark that $O = (0,1,2) \neq (0,0,0)$, the origin; also $O \notin \mathcal{U}$!

With translation symmetry
$\mathrm{T}_3 : P \to P + (2,2,2)$ of path length 3, associate its *quadrant* (union of 12 contiguous sectors)

$$\{(x,y,z) \mid x+y \geq 0 \ \& \ y+z \geq 0 \ \& \ z+x \geq 0\}; \tag{5}$$

$\mathrm{T}_4 : P \to P + (4,0,0)$ of length 4, its 8-sector quadrant (sextant?)

$$\{(x,y,z) \mid x \geq |y| \ \& \ x \geq |z|\}; \tag{6}$$

$\mathrm{T}_6 : P \to P + (4,4,0)$ of length 6, its 4-sector quadrant

$$\{(x,y,z) \mid y \geq |z| \ \& \ x \geq y + |z|\}. \tag{7}$$

T_3 carries the canonical cell to one centred around a cubical centre; together with $\mathcal{O}_3$ it generates the network symmetry group.

2 Height Function

Denote by $\mathrm{ht}(P)$ the *height* of vertex P, the minimum path length from O to P along network edges.

We introduce a mildly indigestible function $h(P)$ on vertices (revealed to equal height by Theorem 5), in terms of $h'(P')$ (equal to mean height over an $\mathcal{O}_3$ orbit):

Definition 1. *For $P' = (x',y',z') \in \mathcal{U}$, let*

$$h'(P') \equiv x' + y'/2 - s(P')/2, \tag{8}$$

where

$$\begin{aligned} s(P') \quad \equiv \quad & (0,1,0,-1) \quad \text{if } y' \bmod 4 = 0,1,2,3, \\ \times \ & (1,0,-1,0) \quad \text{if } x' \bmod 4 = 0,1,2,3. \end{aligned}$$

Now extending this to all sectors,

Definition 2.

$$h(P) \equiv h'(P') + \begin{cases} 0 & \text{if } |x| \geq |y| \geq |z| \\ -\operatorname{sign}(z) & \text{if } |x| \geq |z| \geq |y| \\ -\operatorname{sign}(y) & \text{if } |y| \geq |x| \geq |z| \\ 0 & \text{if } |y| \geq |z| \geq |x| \text{ and } yz \leq 0 \\ -2\operatorname{sign}(z) & \text{if } |y| \geq |z| \geq |x| \text{ and } yz \geq 0 \\ -2\operatorname{sign}(z) & \text{if } |z| \geq |x| \geq |y| \\ -\operatorname{sign}(z) & \text{if } |z| \geq |y| \geq |x| \text{ and } yz \leq 0 \\ -3\operatorname{sign}(y) & \text{if } |z| \geq |y| \geq |x| \text{ and } yz \geq 0 \end{cases} \tag{9}$$

The sector offsets involved above are illustrated in Figure 1, in the form of a section across the x axis, y running top to bottom, z left to right, and origin (beneath) centre. Remark how sectors with a common coordinate plane share equal offsets; also $(x, y, z) \to (-x, y, z)$ is a symmetry, $(x, y, z) \to (x, z, y)$ an antisymmetry.

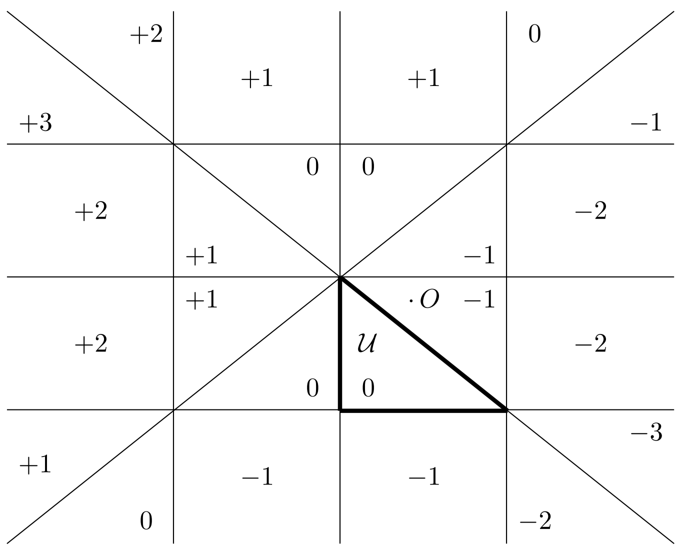

Figure 1: Height offsets by sector: x out, y down, z right, origin central.

Within its quadrant, a translation 'respects' the pretender height function:

Lemma 3.

$$\begin{aligned} h(\mathrm{T}_3 P) &= h(P) + 3 \quad \text{for} \quad P \in \mathrm{T}_3 \text{ quadrant;} \\ h(\mathrm{T}_4 P) &= h(P) + 4 \quad \text{for} \quad P \in \mathrm{T}_4 \text{ quadrant;} \\ h(\mathrm{T}_6 P) &= h(P) + 6 \quad \text{for} \quad P \in \mathrm{T}_6 \text{ quadrant.} \end{aligned}$$

Proof. Within the T_3 quadrant, suppose without loss of generality that $|x| \geq |y| \geq |z|$; then $x \geq y \geq 0$, and via Definition 2

$$\begin{aligned} h(\mathrm{T}_3 P) &= (x+2) + (y+2)/2 + s(x+2, y+2, z+2)/2 \\ &= x + y/2 + s(x,y,z)/2 + 3 = h(P) + 3. \end{aligned}$$

Similarly for T_4, supposing that $|y| \geq |z|$,

$$\begin{aligned} h(\mathrm{T}_4 P) &= (x+4) + y/2 + s(x+4, y, z)/2 \\ &= x + y/2 + s(x,y,z)/2 + 4 = h(P) + 4. \end{aligned}$$

For T_6,

$$\begin{aligned} h(\mathrm{T}_6 P) &= (x+4) + (y+4)/2 + s(x+4, y+4, z)/2 \\ &= x + y/2 + s(x,y,z)/2 + 6 = h(P) + 6. \end{aligned}$$

□

Given a vertex pretending to sufficient height, a useable neighbourhood of it lies entirely within some quadrant:

Lemma 4. *If vertex $P \in \mathcal{U}$ with $h(P) \geq 15$, then P together with its neighbours, and their images under the associated inverse translation T^{-1}, lie within the same quadrant.*

Proof. The components of any neighbour Q vary from those of P by $-1, 0, +1$. Referring to Equation 5 etc. —

Case $y + z > 6$: then $3 \leq y \leq x$. At worst,

$$P = (x, y, z),\ Q = (x, y-1, z-1),$$
$$\mathrm{T_3}^{-1} P = (x-2, y-2, z-2),\ \mathrm{T_3}^{-1} Q = (x-2, y-3, z-3);$$

all remain within the quadrant, including $\mathrm{T_3}^{-1} Q$, since

$$x + y - 5 \geq 0 \ \&\ y + z - 6 \geq 0 \ \&\ z + x - 5 \geq 0.$$

Case $y + z \leq 6$: then $0 \leq y, z \leq 6$, and $x \geq 12$ via Definition 2. At worst,

$$P = (x, y, z),\ Q = (x-1, y+1, z),$$
$$\mathrm{T_4}^{-1} P = (x-4, y, z),\ \mathrm{T_4}^{-1} Q = (x-5, y+1, z);$$

all remain within the quadrant, including $\mathrm{T_4}^{-1} Q$, since

$$x - |y| - 6 \geq 0 \ \&\ x - |z| - 5 \geq 0.$$

□

Theorem 5. $\mathrm{ht}(P) = h(P)$ *for every network vertex P.*

Proof. For $\mathrm{ht}(P) < 15$ the assertion is verified via inspection of an inconveniently extensive table. For $\mathrm{ht}(P) \geq 15$ via a somewhat delicate induction: assume the result for all vertices R with $\mathrm{ht}(R) < \mathrm{ht}(P)$.

First suppose $P \in \mathcal{U}$. P has some neighbour Q nearer to O, so that $\mathrm{ht}(Q) = \mathrm{ht}(P) - 1$; via Lemma 4 all $P, T^{-1}(P), Q, T^{-1}(Q)$ lie in one quadrant, and via Lemma 3 and network symmetry

$$\mathrm{ht}(P) = \mathrm{ht}(Q) + 1 = h(Q) + 1 = h(\mathrm{T}^{-1}Q) + t + 1 = h(\mathrm{T}^{-1}P) + t = h(P),$$

where $t = 3, 4$ for $\mathrm{T} = \mathrm{T}_3, \mathrm{T}_4$ resp.

For any vertex P now, the procedure above may be applied to its sector, employing an appropriate symmetry from $\mathcal{O}_3$, and corresponding height offset from Definition 2. $\square$

3 Spherical Content Function

Consider now the content of a 'sphere' in the corresponding metric, also the 'vertex coordination sequence' of the tiling: that is, the number of vertices $S(n)$ at given height n from O.

We introduce functions (there are more to come!) for the content of a 'sphere' of given height n, and of the 'armillary sphere' where it meets the coordinate planes, and of their restrictions to the canonical sector:

Definition 6.

$$\begin{aligned}
S(n) &\equiv \#(P \mid \mathrm{ht}(P) = n); \\
\bar{S}(n) &\equiv \#(P \mid \mathrm{ht}(P) = n \;\&\; xyz = 0); \\
S_2(n) &\equiv \#(P \in \mathcal{U} \mid \mathrm{ht}(P) = n); \\
\bar{S}_1(n) &\equiv \#(P \in \mathcal{U} \mid \mathrm{ht}(P) = n \;\&\; xyz = 0);
\end{aligned}$$

$n =$	0	1	2	3	4	5	6	7	8	9	10	11	12
$\bar{S}(n) =$	1	4	8	12	16	20	24	28	32	36	40	44	48
$S(n) =$	4	10	20	34	52	74	100	130	164	202	244	290	340

Figure 2: Table of network sphere content

Lemma 7. *There are finitely many constants a_j, b_j, c_j such that for all n,*

$$\begin{aligned}
\bar{S}(n) &= \sum_j a_j \bar{S}_1(n+j), \\
S(n) &= \sum_j b_j \bar{S}_1(n+j) + \sum_j c_j S_2(n+j).
\end{aligned}$$

Proof. Firstly notice that via Equation 2 the only tiling vertices on the boundary of a sector are those interior to a facet on a coordinate plane, since the other two planes are diagonal.

Now via Definition 9 and Theorem 5, for $n > 0$,

$$\begin{aligned}
\bar{S}(n) &= 6\bar{S}_1(n) + 3\bar{S}_1(n-1) + 3\bar{S}_1(n+1) + \bar{S}_1(n+2) + \bar{S}_1(n-2) \\
&\quad + \bar{S}_1(n+3) + \bar{S}_1(n-3) + 2\bar{S}_1(n+1) + 2\bar{S}_1(n-1) \\
&\quad + 2\bar{S}_1(n+2) + 2\bar{S}_1(n-2); \\
S(n) &= 2\big(6S_2(n) + 3S_2(n-1) + 3S_2(n+1) + S_2(n+2) + S_2(n-2) \\
&\quad + S_2(n+3) + S_2(n-3) + 2S_2(n+1) + 2S_2(n-1) \\
&\quad + 2S_2(n+2) + 2S_2(n-2)\big) - \bar{S}(n);
\end{aligned}$$

the final term corrects for the boundary being counted double, and is then substituted via the first equation. ☐

Theorem 8.

$$\bar{S}(n) = \begin{cases} 1 & \text{if } n = 0, \\ 4n & \text{if } n > 0. \end{cases}$$

$$S(n) = \begin{cases} 1 & \text{if } n = 0, \\ 2(n^2+1) & \text{if } n > 0; \end{cases}$$

Proof. $P = (x, y, z)$ will be restricted implicitly to vertices at height n in sector $\mathcal{U}$. Also assume $n > 6$, avoiding special values for $n \leq 0$. Lemma 3 is employed without reference, noting $\mathcal{U}$ is a subset of all relevant quadrants. A leaning tower of further subsidiary functions follows:

Firstly via $P \to \mathrm{T_4}^{-1}P$ from Equation 5 etc.,

$$\bar{S}_1(n) \equiv \#(P \mid 0 = z \leq y \leq x) = \bar{S}_1(n-4) + \bar{S}_0(n);$$

where via $P \to \mathrm{T_6}^{-1}P$,

$$\bar{S}_0(n) \equiv \#(P \mid x - 4 < y \leq x) = \bar{S}_0(n-6) = \text{constant},$$

depending on n mod 6, n mod 4. Hence the $\bar{S}_1(12i + j)$ are polynomials linear in i, depending only on $j = n$ mod 12.

Similarly via $P \to \mathrm{T_3}^{-1}P$,

$$S_2(n) \equiv \#(P \mid 0 \leq z \leq y \leq x) = S_2(n-3) + S_1(n);$$

where via $P \to \mathrm{T_6}^{-1}P$,

$$S_1(n) \equiv \#(P \mid 0 \leq z < 2) = S_1(n-6) + S_0(n);$$

where via $P \to \mathrm{T_4}^{-1}P$,

$$S_0(n) \equiv \#(P \mid 0 \leq z < 2 \;\&\; z \leq y < 4) = S_0(n-4) = \text{constant},$$

depending on n mod 3, n mod 6, n mod 4. Hence the $S_2(12i+j)$ are polynomials quadratic in i, depending only on $j = n$ mod 12.

For via Lemma 7, both $\bar{S}(12i+j), S(12i+j)$ are also such sets of polynomials; and by inspection of Figure 2, each set reduces (mysteriously) to the single polynomial in $n > 0$ shown. □

4 Discussion

Coordination sequences for networks associated with lattices in Euclidean d-space are established in [3] and [2] for numerous classical cases, using general group-theoretic methods. However, an explicit expression for the coordination sequence $S(n)$ in Theorem 8 — case $d = 3$ of Equation (3.43) in [3] — was designated conjectural, and has since been dubbed by one author 'really tricky'.

The approach used above relies on two ideas. One is intuitively obvious: for all vertices P lying sufficiently far from the height zero vertex O in the direction of translation T, translation must respect height, in the sense that $\mathrm{ht}(\mathrm{T}\,P) = \mathrm{ht}(P) + t$ for constant t. As a result, the sphere of height $n + t$ is the union of translations of overlapping segments of the sphere of height n. The difficulty comes in quantifying regions in which this respectful behaviour can be guaranteed, for some neighbourhood of P sufficient to facilitate induction: it is overcome by overlapping adjacent quadrants so far, that P cannot avoid lying well inside (at least) one.

Given the explicit expression Definition 2 for height, it would be feasible (though tedious) to compute content $S(n)$ as the number of solutions of the compound linear equation $h(x, y, z) = n$. However, it is not actually necessary to know $\mathrm{ht}(P)$ in order to find $S(n)$; only Lemma 3, that outside some finite initial region, translation respects height.

References to 'inspection' are in practice made tongue-in-cheek. Frequent resort to a computer is inevitable if the proof is to be fully checked, starting with tabulation of $\mathrm{ht}(P) \leq 20$ via some tree-search algorithm, and implementation of $h(P)$, and extending either to compute $S(n)$ by enumeration.

Various features of the proofs merit further discussion.

(A) The coordinates employed above for sodalite are special to dimension $d = 3$, and do not generalise to other spaces. Conventional coordinates for d-space sodalite (aka 'honeycomb of permutohedra') are sketched in [1].

(B) The proof of Lemma 7 and Theorem 8 involved establishing existence of moderately complicated linear combinations and polynomial sets; however, their actual coefficients are ultimately irrelevant.

(C) Indeed, if only we could be certain in advance that the the final result in Theorem 8 would be a quadratic polynomial (or more generally, ultimately satisfied some linear recurrence with constant coefficients and known order), only minor routine computation would subsequently be required.

(D) Although in this instance height $\mathrm{ht}(P)$ is represented by expression $h(P)$ for all $\mathrm{ht}(P) \geq 0$, content $S(n)$ takes special values unless $n = \mathrm{ht}(P) \geq 1$. In

other situations it may be nontrivial to establish a lower bound on height above which the corresponding functions behave well.
(E) Larger still is the bound — $\mathrm{ht}(P) \geq 15$ in Lemma 4 — required to ensure that height is respected by inverse translation, below which we are obliged to verify a result via inspection. Unfortunately this bound depends in a complicated fashion on the geometric interaction between translations, and may well grow rapidly with dimension.
(F) The quadrant associated with a translation T would in general be the union of those sectors having an edge along its axis. This rule is subverted by T_3 in Equation 5, which spills over into a further 6 adjacent sectors. The effect is to simplify the proof of Lemma 4, which otherwise would otherwise involve (dimension) $d = 3$ translations including T_6.
(G) The proof of Lemma 7 would be considerably complicated by any necessity to consider vertices lying on lower-dimensional boundary elements (here edges, corner) of a sector.
(H) Assignment of coordinates labelling vertices is a delicate matter, governed by availability of convenient generators for the symmetry group. In particular, it may be inadvisable to locate vertex O at origin $(0, 0, 0)$, or indeed to assign a vertex to the origin at all: instead the frame should reflect the full point-group of the network.

All in all there appear to remain considerable obstructions to recasting our approach as an abstract theorem applicable to a class of networks, analogous to Theorems 2.4 and 2.9 of [3]. In the meantime, the method has been successfully applied to the snub-square and knight's move networks.

References

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